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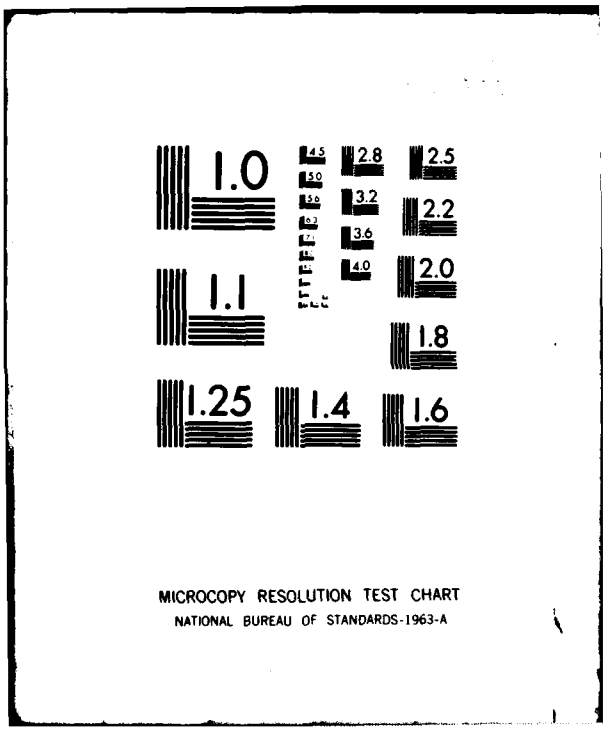
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THEORY OF ELECTRONIC, ATOMIC, AND MOLECULAR CALCULATIONS

R. K. Nesbet

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San Jose, California 95193

Response to Summary Questionaire,

ONR Contract No. N00014-79-C-0406

1. Principal Investigator:

   Robert K. Nesbet

2. Contract Description:

   The general subject matter is atomic and molecular scattering theory.

3. Scientific Problem:

The new methods to be developed have many specific applications. Quantitative calculations of atom-molecule and of electron-molecule scattering cross sections are required for verification of qualitative interpretations of complex experimental data, for prediction of fundamental rate constants that may not at present be directly measurable, and for provision of accurate standard cross sections for calibrating experimental data.

4. Scientifc and Technical Approach:

The general approach is to develop computational methods that are quantitative in the sense of being based on the exact formal theory of the processes considered, and are practicable, in the sense of being capable of implementation on digital computers at the present level of technology. For atom-molecule scattering, a new method is being developed that extends a recent theory of the action constants of nonseparable dynamical systems to collision problems. For electron-molecule scattering, a new method for treating vibrational and rotational excitation has been developed, formal theoretical relations needed in detailed applications of this method are being derived, and a new variational approach to quantitative fixed-nuclei calculations is being planned for practical implementation.

5. Progress:

A. Fourier transform method for molecular collisions

The technique of imposing an infinite potential barrier, to convert collision dynamics into bound motion, has been tested for simple model problems. The technique of converting Percival's nonlinear equations to iterated inhomogeneous linear equations, with quadratic convergence, has also been tested. The general methodology has been tested for examples of double-well potential functions. The conceptual basis of reactive collision problems in this formalism has been characterized, requiring multiple-valued invariant toroids in which different arrangement sheets are connected across branch cuts.

B. Multichannel scattering theory

The formalism of a generalized hybrid scattering theory has been

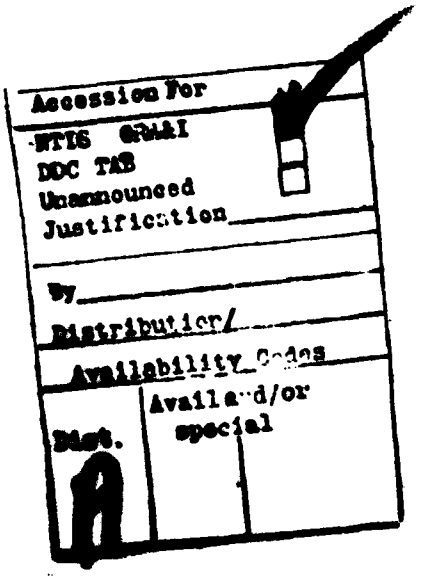
developed, making use of the Green's function, appropriate to exact solution of a multichannel model scattering problem. The resulting Lippmann-Schwinger equation gives an expression for the incremental reactance matrix (K-matrix) in terms of the residual multichannel potential function or Hamiltonian. This result can be used directly, in a distorted-wave approximation, valid when the residual potential is weak, or indirectly, through a multichannel Schwinger variational principle, for quantitative calculations.

C. Theory of multichannel threshold structures

A new formal analysis of multichannel threshold theory has been carried out, leading to matrix formulas that separate background scattering from the effects of pole singularities. This separation is required for application in electron-molecule scattering.

D. Electron-molecule scattering

The EMA method for vibrational excitation in electron-molecule scattering has been extended to provide a new theory of dissociative attachment and of the inverse detachment process.



6. Publications

6.1. R. K. Nesbet and D. C. Clary, "Fourier Transform Method for the Classical Trajectory Problem", J. Chem. Phys. 71, 1372 (1979).

6.2. D. C. Clary and R. K. Nesbet, "Application of a Dynamical S-Matrix Method to the Three-Dimensional H + H_2 Exchange Reaction", J. Chem. Phys. 71, 1101 (1979).

6.3. R. K. Nesbet, "Accurate e^--He Cross Sections Below 19eV", J. Phys. B12, L243 (1979).

6.4. R. K. Nesbet, "Variational Calculations of Accurate e^--He Cross Sections Below 19eV", Phys. Rev. A20, 58 (1979).

6.5. D. C. Clary, "Semiclassical Method for the Determination of Potential Energy Functions of Polyatomic Molecules", Chemical Physics 41, 387 (1979).

6.6. R. K. Nesbet, "Energy-Modified Adiabatic Approximation for Scattering Theory", Phys. Rev. A19, 551 (1979).

6.7. R. K. Nesbet and J. Bruinsma, "Fourier Transform Method for Collision Dynamics: Reactive Collisions", Abstract, First West Coast Theoretical Chemistry Conference (San Jose, California, 1979), p. 18.

6.8. J. Bruinsma and R. K. Nesbet, "Fourier Transform Method for Collision Dynamics: Model Studies", Abstract, First West Coast Theoretical Chemistry Conference (San Jose, California, 1979), p. 38a.

6.9. R. K. Nesbet, "Theory of Electron Scattering Using a Hybrid Schwinger Formalism", Abstract, Bull. Am. Phys. Soc. 24, 1189 (1979).

6.10. R. K. Nesbet, "Multichannel Threshold Structures in Scattering

Theory,", J. Phys. B13), xxx (1980).

6.11. R. K. Nesbet, "Resonance and Threshold Effects in Low Energy Electron Scattering by Molecules", Proceedings, Workshop in Molecular Physics and Quantum Chemistry (Wollongong, NSW, Australia, February, 1980).

6.12. R. K. Nesbet, "Surprisal Theory," in Theoretical Chemistry Advances and Perspectives, edited by H. Eyring and D. Henderson (Academic Press, New York, 1980).

7. Extenuating circumstances: None

8. Unspent funds: Not expected

9. Graduate students: None

10. Other Federal grant or contract support: None